Crossing points in specific-heat curves of the asymmetric Hubbard model

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The phenomenon of the crossing points in specific-heat curves $C(T,U)$ versus T of the one-dimensional half-filled-band asymmetric Hubbard model is investigated within the method of small-cluster exact-diagonalization calculations with extrapolation techniques to the infinite chain. A definite region where the crossing points occur is found to exist in a certain range of system parameters R (relative magnitude of the transfer integrals) and U (local interaction). We identify an association between crossing point occurrence and gradual localization of fermions.

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The literature reveals quite a number of materials where the specific-heat curves $C(T,X)$ versus T, when plotted for different values of a second thermodynamic variable X, intersect at one or even two well-defined nonzero temperatures. For example, crossing points are observed by changing the magnetic field $(X=B)$ in heavy fermion compounds such as $CeCu_{5.5}Au_{0.5}$ (Ref. 1) and $Nd_{2-x}Ce_xCuO_4$,[2] by changing the pressures $(X=P)$ in $CeAl_3$ (Ref. 3) and in the normal liquid ^3He.[4]

Crossings of the specific-heat curves are also observed in the simplest lattice model for correlated electrons, the Hubbard model.[5] At half filling, the curves $C(T,U)$ versus T, where U is the local interaction, always cross at two temperatures. This is observed, for example, in the case of the model with nearest-neighbor hopping in $d=1$,[6,7] $d=2$,[8] and $d=\infty$,[9] as well as for long-range hopping in $d=1$.[10] Furthermore, crossing is found in $d=1$ when a magnetic field B is changed at constant U.[11]

Recently, Vollhardt *et al.*[12,13] developed an ample analysis of the characteristic crossing points in specific-heat curves of a general class of Hubbard models. That study established a quantitative explanation, within second order perturbation theory and certain generalized susceptibilities of the system, of why specific-heat curves cross at all, of how wide is the region where the curves cross, and the value C_+ of the specific-heat curves at their high-temperature crossing point T_+. Mishra and Sreeram,[14] studing the normal phase of liquid ^3He and the heavy fermion systems $CeAl_3$ and UBe_{13} within the spin fluctuation theory, show that crossing of specific heat is related to the possibility of existence of a quantum critical point. Macedo *et al.*[15] show that the one-dimensional half-filled-band Falicov-Kimball model does not exhibit the crossing point of the specific heat curves.

The fact that the one-dimensional half-filled-band Falicov-Kimball model does not show the crossing point[15] and that the one-dimensional half-filled-band Hubbard model does[12,13] suggests the question of which physical phenomenon is associated with the crossing point that is present in the Hubbard model and not present in the Falicov-Kimball model. In order to contribute to a better understanding of the physical phenomenon associated with the crossing points in specific-heat curves of simple lattices models for correlated fermions, we study the temperature dependence of the specific heat of the one-dimensional half-filled-band asymmetric Hubbard model.[16–18] This model represents a correlated fermion system in which two species of spinless particles exist, called electrons and ions. Both electrons and ions are allowed to jump between sites. The Coulombian energy for two particles of the same sort is too large to allow them to occupy the same site, but the energy remains finite and equal to U for an electron and an ion on the same site.

The asymmetric Hubbard model, in its one-dimensional form for a lattice of N sites, can be written as

$$H=-\sum_j (t_e d_j^\dagger d_{j+1}+t_i f_j^\dagger f_{j+1}+\mathrm{H.c.})+U\sum_j n_{d_j} n_{f_j}, \tag{1}$$

where $d_j^\dagger(d_j)$ and $f_j^\dagger(f_j)$ are, respectively, the creation (annihilation) operators for the electrons and ions at site j, and the hopping parameters t_e and t_i refer to electrons and ions, respectively. The number of electrons (ions) at site j is denoted as $n_{d_j}=d_j^\dagger d_j$ $(n_{f_j}=f_j^\dagger f_j)$.

Clearly the asymmetric Hubbard model (1) reduces to the usual Hubbard model for $t_e=t_\uparrow=t_i=t_\downarrow=t$ and to the spinless Falicov-Kimball model[19] for $t_i=0$. Our study was developed for several values of parameters U and $R\equiv t_i/t_e$ (the relative magnitude of the ion transfer integral to electron transfer integral). The values of the parameter R extend from 0 to 1. For $R=0$ the asymmetric Hubbard model becomes the spinless Falicov-Kimbal model, and for $R=1$ the asymmetric Hubbard model corresponds mathematically to the simple Hubbard model.

The asymmetric Hubbard model is one of the simplest two-band models which are believed to describe many essential physical properties of strongly correlated systems such as superconducting cuprates, valence fluctuating, or heavy fermion systems.[17] In our work we used small-cluster exact-diagonalization calculations with the application of the grand canonical ensemble and of extrapolation techniques to the infinite chain.[7,15,20]

The phenomenon of the crossing point of the specific-heat curves of the one-dimensional half-filled-band asymmetric Hubbard model occurs in the range of values of $U, 0\leqslant U \leqslant U_S$, where the superior limit U_S in the case of the simple Hubbard model $(R=1)$ corresponds to bandwidth $U_S=4t$. Figure 1 shows examples of the behavior of the specific-heat curves in two distinct values of R. The curves $C(T,U)$ ver-

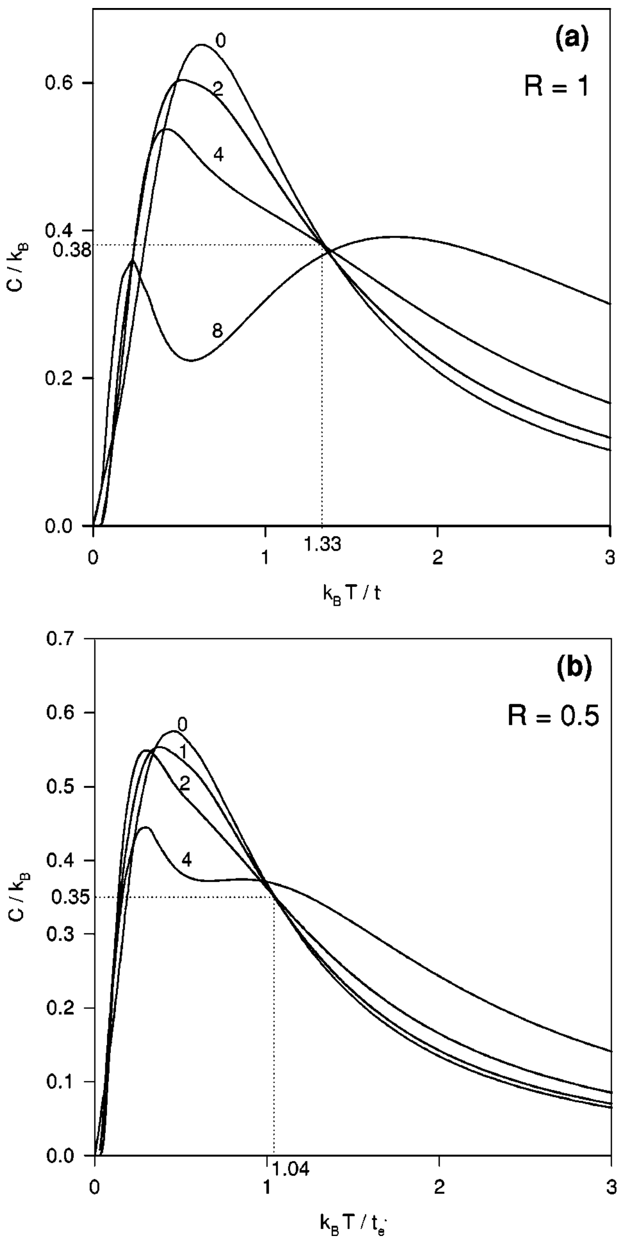

FIG. 1. Specific heat for the one-dimensional half-filled-band asymmetric Hubbard model. (a) $R=1$, where $k_BT_+=1.33t$, $C_+=0.38k_B$, and $U_S=4t$. (b) $R=0.5$, where $k_BT_+=1.04t_e$, $C_+=0.35k_B$, and $U_S=2.1t_e$. The numbers labeling the curves refer to the values of U/t_e.

sus T with values of U in the range $0 \leqslant U \leqslant U_S$ present only one peak, while those ones with $U>U_S$ present two peaks, indicating an association between crossing point occurrence and gradual localization of fermions.[15]

For $U>U_S$ the two peaks reflect a rearrangement of the fermionic structure in the system. The low-temperature peak arises due to low-lying collective excitations, while the high-temperature broad peak comes from single-particle excitations (or charge transfer excitations). This conclusion is supported by the behavior of the correlation functions

$$L_\delta(T)=\frac{1}{4N}\sum_j \langle \sigma_j \sigma_{j+\delta}\rangle, \tag{2}$$

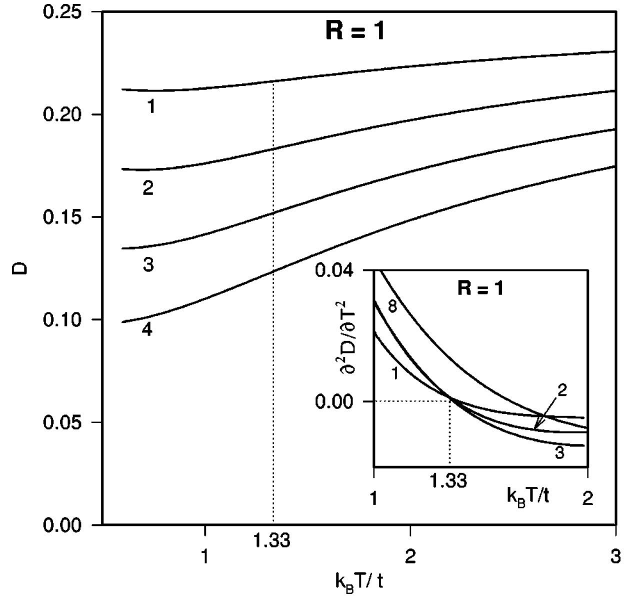

FIG. 2. Behavior of the number of doubly occupied sites in the system. The value $k_BT_+/t=1.33$ identifies the turning point for $R=1$. The inset shows $\partial^2 D/\partial T^2$ versus T. The numbers labeling the curves refer to the values of U/t.

where $\sigma_j=n_{fj}-n_{dj}$ is the operator for the difference between the ion and electron numbers in the site j, by means of the analysis of the change of curvature of the correlation functions following the method developed in Ref. 15.

Our result show that the value of U_S decreases with the decreasing of R. This result expresses the importance of the crescent ionic immobility that occur with the reduction of the value of R, which makes the rearrangement of the fermionic

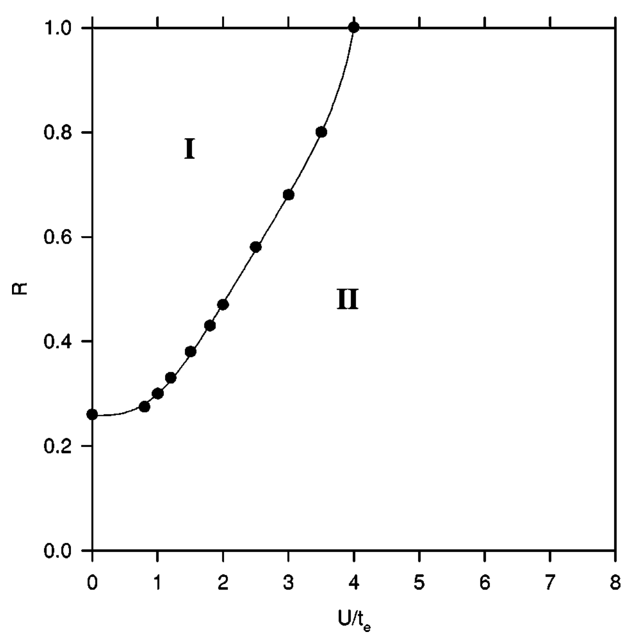

FIG. 3. Diagram indicating the region of pairs (R,U) where crossing point phenomenon takes place in the one-dimensional asymmetric Hubbard model (region I). In region II there is no crossing point.

structure in the system as U increases easy. In the one-dimensional Hubbard model the bandwidth of both spins is $4t$, thus for $U<4t$, double particle occupation is possible in a site having a lower energy than the state in single occupation on the top of the band. In a chain of asymmetric Hubbard model the bandwidth of electrons is $4t_e$, while the bandwidth of ions is $4Rt_e$. Thus, for any value of $U>U_S$, the double occupation of fermions leads to an energy of the system larger than the one that would occur in the case of simple occupation in the maximum level of energy of a fermion.

At the crossing temperature T_+, the specific heat is independent of U, then[12]

$$\left.\frac{\partial C}{\partial U}\right|_{T_+} = T_+ \left.\frac{\partial^2 D}{\partial T^2}\right|_{T_+} = 0, \tag{3}$$

where D is the number of doubly occupied sites in the system. Thus the crossing points occur where $D(T,U)$ versus T has a turning point at T_+ in the range $0 \leqslant U \leqslant U_S$. Figure 2 illustrates the behavior of D and $\partial^2 D/\partial T^2$ versus T.

The characteristic parameters of the crossing point phenomenon are only dependent of R, i.e., $T_+ = T_+(R)$, $C_+ = C_+(R)$, and $U_S = U_S(R)$. The relation among these different parameters can be expressed in the diagram of the region of R versus U, as shown in Fig. 3, that defines the range of pairs (R,U) in which crossing points of the curves $C(T,U)$ versus T take place. There is an inferior limit of the parameter $R(R_I = 0.26)$, below which $U_S = 0$, i.e., no crossing point phenomenon occurs. R_I is the minimum ratio between the bandwidths of ions and electrons where it still is possible to occur the crossing points.

In summary, we have studied the phenomenon of the crossing points in specific-heat curves $C(T,U)$ versus T of the one-dimensional half-filled-band asymmetric Hubbard model for different relative magnitudes of the transfer integrals R. We determine the diagram of the region $R \times U$ where the crossing points $(0 \leqslant U \leqslant U_S)$ take place. The results show that the examined asymmetric Hubbard model exhibits the crossing points in a definite region of the parameters U and R corresponding to the region where the specific heat curves exhibit only one peak. The definite region encompasses the limits of the simple Hubbard model $(R=1)$, while it excludes the limit of the spinless Falicov-Kimball model $(R=0)$. The crossing point temperatures are connected to the gradual localization of fermions in the system.

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